

Supporting Information

Synthesis and Ligand Non-Innocence of Thiolate-Ligated (N₄S) Iron(II) and Nickel(II) Bis(imino)pyridine Complexes

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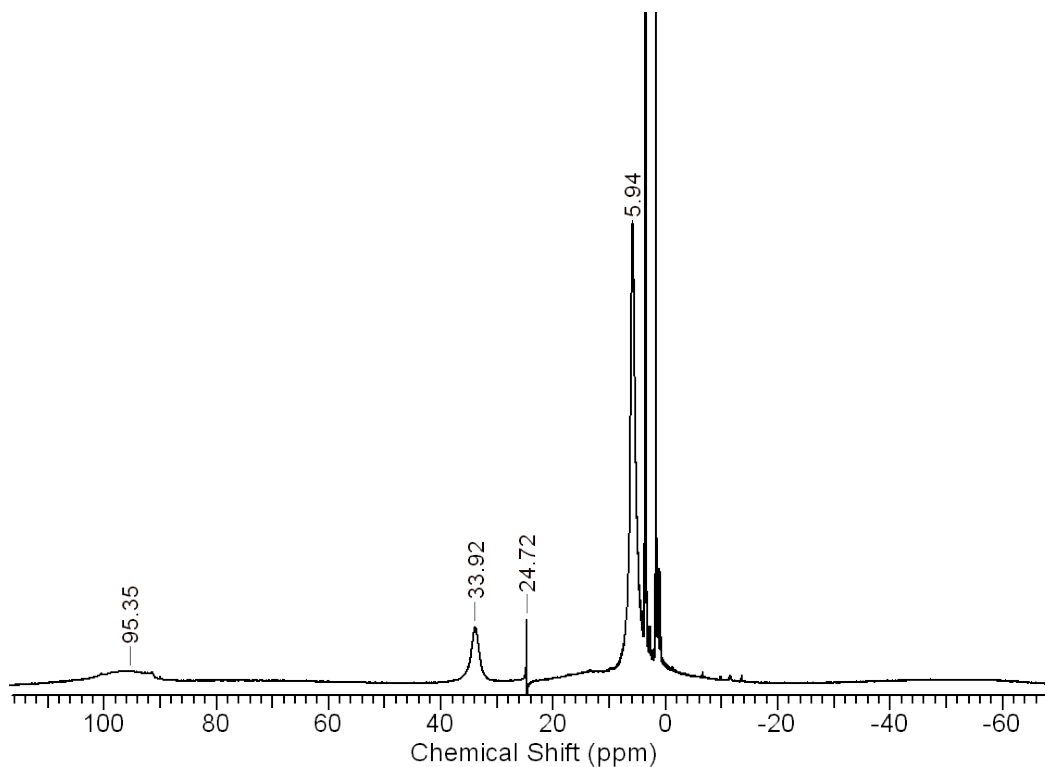


Figure S1. ^1H NMR spectrum of **4** (25 °C, $\text{THF-}d_8$).

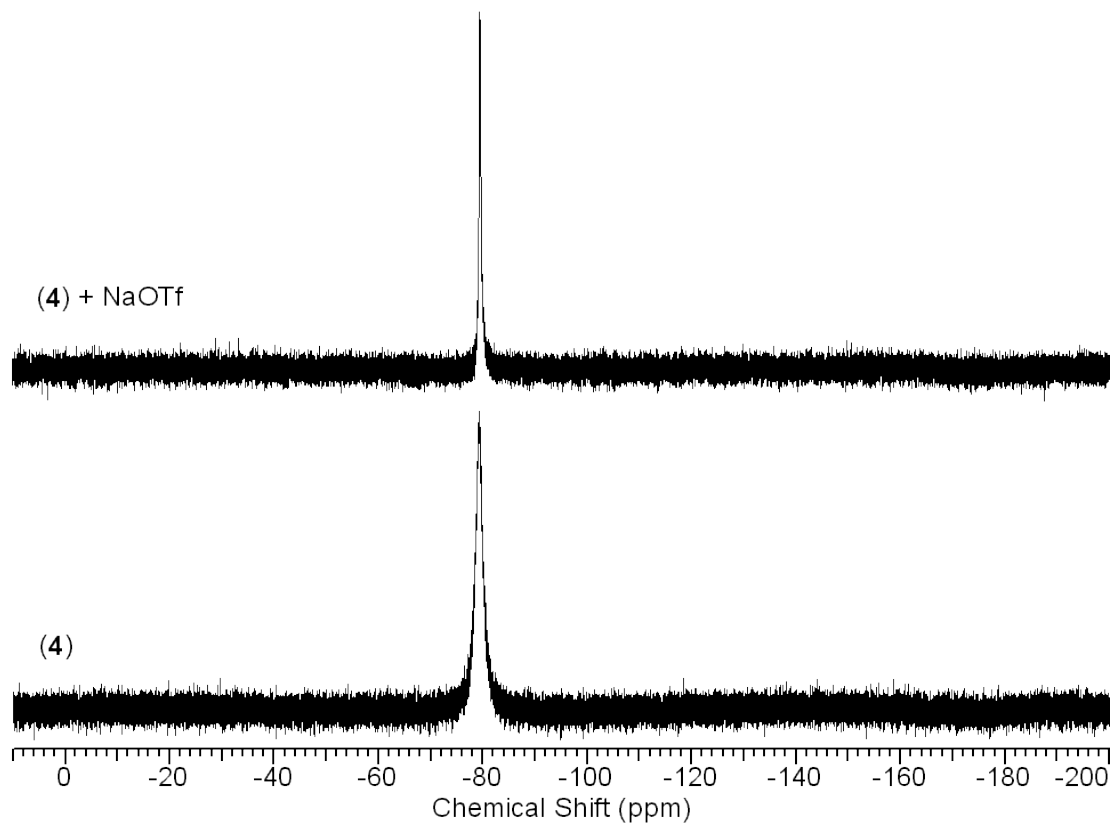


Figure S2. ^{19}F NMR spectra (25 °C, $\text{THF-}d_8$) of crystalline **4**• $2\text{Et}_2\text{O}$ with NaOTf impurity (bottom) and the same sample with added NaOTf (top).

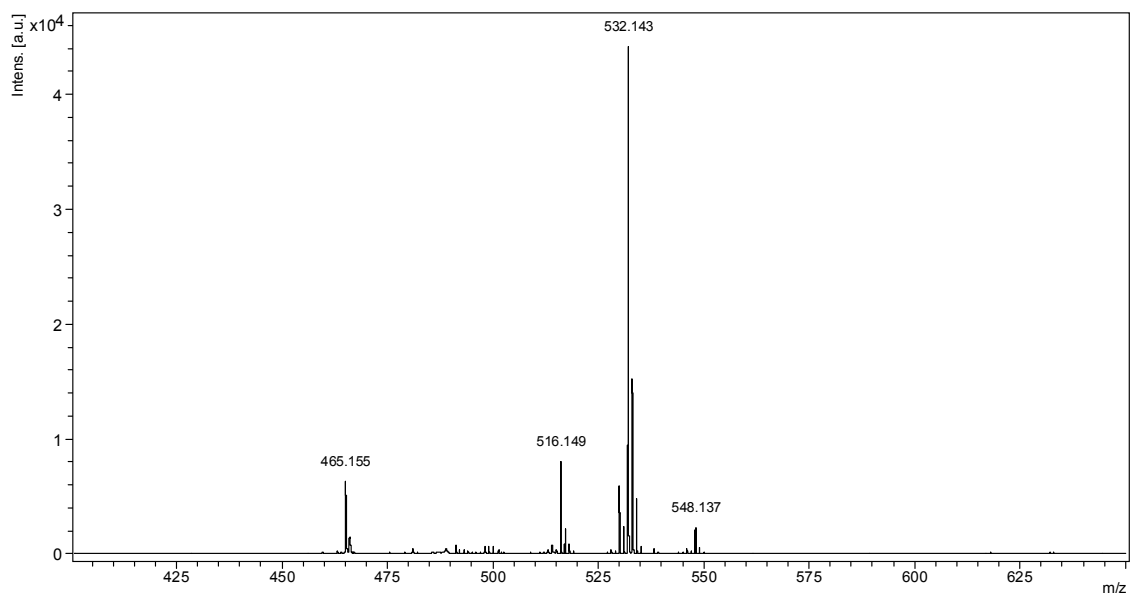


Figure S3. LDIMS(+) of **2** + excess O_2 after 24 h in CH_2Cl_2 . m/z = 516.15 ($[2 + 20 - py - OTf]^+$), 532.14 ($[2 + 30 - py - OTf]^+$).

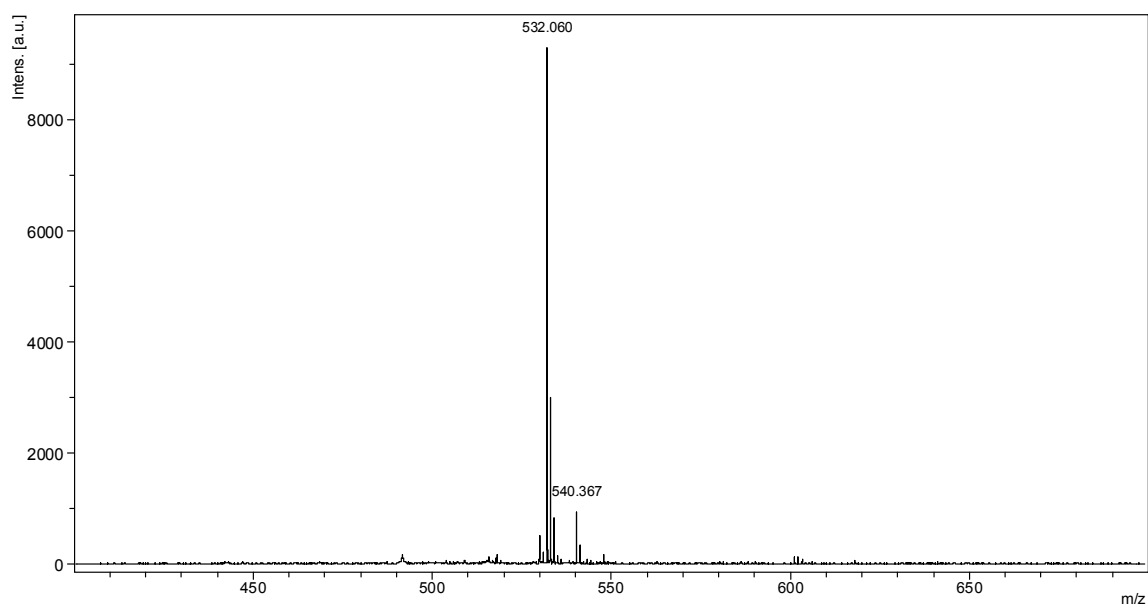


Figure S4. LDIMS(+) of **3** + excess O_2 after 24 h in CH_2Cl_2 . m/z = 532.06 ($[3 + 30 - DMAP - OTf]^+$).

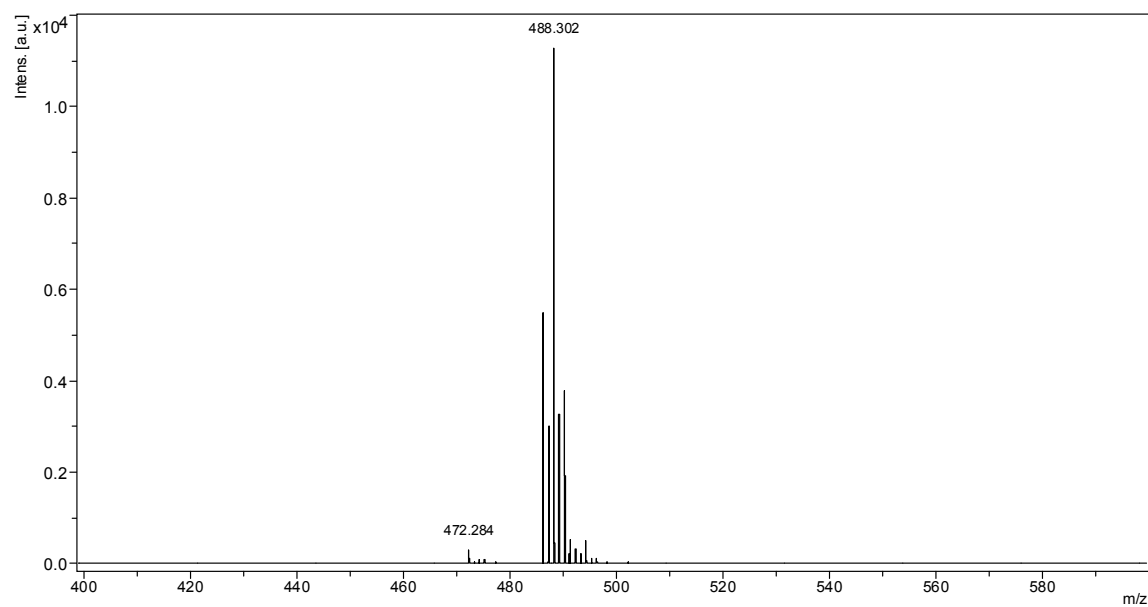


Figure S5. LDIMS(+) of **5** + excess Na/Hg, followed by exposure to excess O_2 in Et_2O . m/z = 488.3 ($[5 - BF_4]^+$).

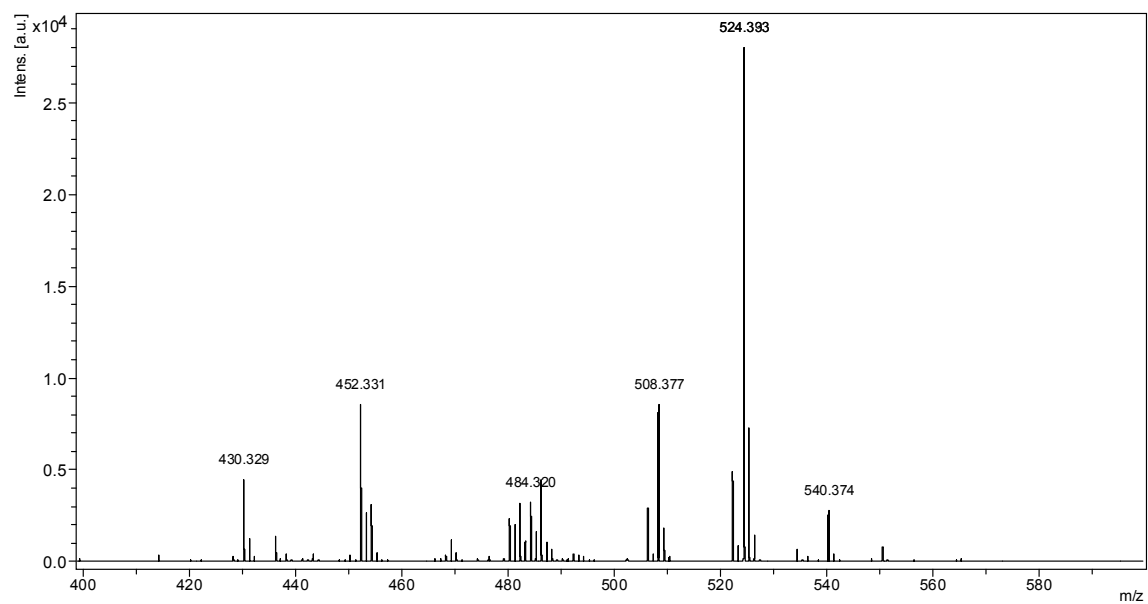


Figure S6. LDIMS(+) of **4** + excess O_2 in Et_2O . m/z = 484.3 ($[3 - DMAP - OTf]^+$), m/z = 508.3 ($[LN_3SOFe^{III}-O-Fe^{III}SOLN_3]^{2+}$), m/z = 524.4 ($[LN_3SO_2Fe^{III}-O-Fe^{III}SO_2LN_3]^{2+}$), and m/z = 540.4 ($[LN_3SO_3Fe^{III}-O-Fe^{III}SO_3LN_3S]^{2+}$).

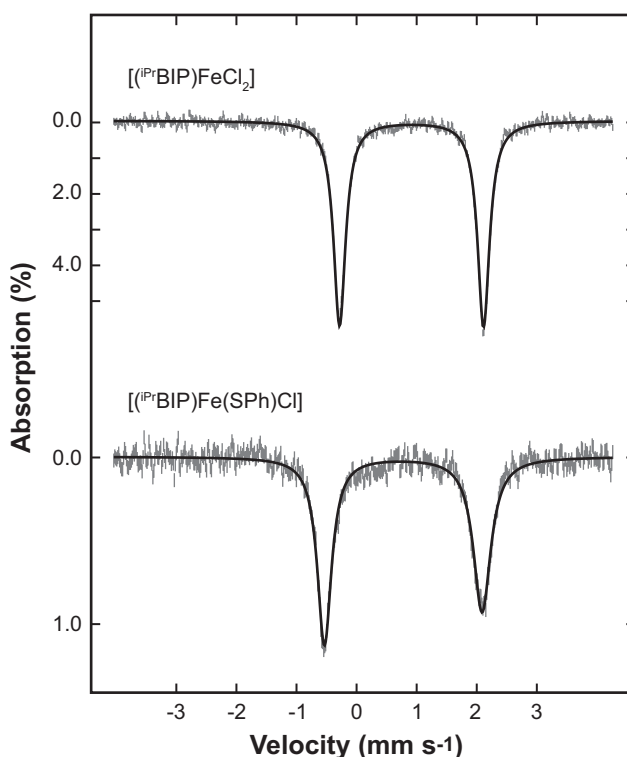


Figure S7. ^{57}Fe Mössbauer spectra of $[(i\text{PrBIP})\text{FeCl}_2]$ and $[(i\text{PrBIP})\text{Fe}(\text{SPh})\text{Cl}]$ measured at 5.6 K and with an applied field of 47 mT parallel to the γ -rays. Both spectra can be fitted to sharp quadrupole doublets with parameters given in Table 4. The starting material $[(i\text{PrBIP})\text{FeCl}_2]$ was measured for completeness, although it was previously reported [ref 40].

X-ray Crystallography

All reflection intensities were measured at 110(2) K using a KM4/Xcalibur (detector: Sapphire3) with enhance graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$) under the program CrysAlisPro (Versions 1.171.33.48, 1.171.33.55, and 1.171.34.49, Agilent Technologies). The program CrysAlisPro (Versions 1.171.33.48, 1.171.33.55, and 1.171.34.49, Agilent Technologies) was used to refine the cell dimensions. Data reduction was done using the program CrysAlisPro (Versions 1.171.33.48, 1.171.33.55, and 1.171.34.49, Agilent Technologies). The structures were solved with the program SHELXS-97¹ and were refined on F^2 with SHELXL-97.¹ Analytical numeric absorption corrections based on a multifaceted crystal model were applied using CrysAlisPro (Versions 1.171.33.48, 1.171.33.55, and 1.171.34.49, Agilent Technologies). The temperature of the data collection was controlled using the system Cryojel (manufactured

by Oxford Instruments). The H-atoms were placed at calculated positions using the instructions AFIX 13, AFIX 23, AFIX 43 or AFIX 137 with isotropic displacement parameters having values 1.2 or 1.5 times U_{eq} of the attached C atoms.

Crystal structure of 2: The structure is ordered. The crystal which was mounted on the diffractometer was twinned. The twin relationship was resolved using the program TwinRotMat from Platon;² the two twinned components are related by a twofold axis along the $\mathbf{a}^*$ direction. The structure is also racemically twinned. The fractional contribution of the three components (*i.e.*, the BASF batch scale factor) refined to 0.185(8), 0.546(13), 0.212(13). $F_w = 712.62$, dark brown thick plate, $0.41 \times 0.20 \times 0.10$ mm³, monoclinic, Pc (no. 7), $a = 17.6133(5)$, $b = 10.4554(2)$, $c = 18.8663(4)$ Å, $\beta = 105.548(3)^\circ$, $V = 3347.17(13)$ Å³, $Z = 4$, $D_x = 1.414$ g cm⁻³, $\mu = 0.632$ mm⁻¹, abs. corr. range: 0.632–0.827. 26684 Reflections were measured up to a resolution of $(\sin \theta/\lambda)_{\max} = 0.59$ Å⁻¹. 11193 Reflections were unique ($R_{\text{int}} = 0.0652$), of which 8793 were observed [$I > 2\sigma(I)$]. 844 Parameters were refined with 282 restraints. $R1/wR2$ [$I > 2\sigma(I)$]: 0.0471/0.1068. $R1/wR2$ [all refl.]: 0.0661/0.1136. $S = 0.993$. Residual electron density found between -0.75 and 0.78 eÅ⁻³.

Crystal structure of 3: The structure is ordered. $F_w = 755.69$, black plate, $0.49 \times 0.36 \times 0.07$ mm³, monoclinic, $C2/c$ (no. 15), $a = 30.8054(16)$, $b = 10.2837(2)$, $c = 25.181(4)$ Å, $\beta = 116.305(6)^\circ$, $V = 7151.1(12)$ Å³, $Z = 8$, $D_x = 1.404$ g cm⁻³, $\mu = 0.596$ mm⁻¹, abs. corr. range: 0.802–0.962. 29265 Reflections were measured up to a resolution of $(\sin \theta/\lambda)_{\max} = 0.62$ Å⁻¹. 7007 Reflections were unique ($R_{\text{int}} = 0.0400$), of which 5442 were observed [$I > 2\sigma(I)$]. 450 Parameters were refined. $R1/wR2$ [$I > 2\sigma(I)$]: 0.0314/0.0756. $R1/wR2$ [all refl.]: 0.0474/0.0796. $S = 1.026$. Residual electron density found between -0.46 and 0.30 eÅ⁻³.

Crystal structure of 4: The structure is ordered. The asymmetric unit contains one molecule of Fe complex and two uncoordinated diethyl ether solvent molecules. $F_w = 754.86$, dark brown lath, $0.49 \times 0.21 \times 0.07$ mm³, monoclinic, $P2_1/c$ (no. 14), $a = 19.5713(4)$, $b = 10.9561(2)$, $c = 19.7953(3)$ Å, $\beta = 103.7517(18)^\circ$, $V = 4122.94(13)$ Å³, Z

= 4, $D_x = 1.216 \text{ g cm}^{-3}$, $\mu = 0.457 \text{ mm}^{-1}$, abs. corr. range: 0.871–0.977. 37056 Reflections were measured up to a resolution of $(\sin \theta/\lambda)_{\max} = 0.61 \text{ \AA}^{-1}$. 7886 Reflections were unique ($R_{\text{int}} = 0.0433$), of which 6329 were observed [$I > 2\sigma(I)$]. 472 Parameters were refined. $R1/wR2$ [$I > 2\sigma(I)$]: 0.0379/0.0823. $R1/wR2$ [all refl.]: 0.0542/0.0879. $S = 1.035$. Residual electron density found between -0.30 and $0.47 \text{ e \AA}^{-3}$.

Crystal structure of 5: The structure is ordered. $F_w = 659.05$, red plate, $0.56 \times 0.33 \times 0.07 \text{ mm}^3$, monoclinic, $P2_1/c$ (no. 14), $a = 15.13933(17)$, $b = 13.80648(15)$, $c = 13.94752(16) \text{ \AA}$, $\beta = 95.0548(10)^\circ$, $V = 2903.98(6) \text{ \AA}^3$, $Z = 4$, $D_x = 1.507 \text{ g cm}^{-3}$, $\mu = 0.974 \text{ mm}^{-1}$, abs. corr. range: 0.728–0.951. 39899 Reflections were measured up to a resolution of $(\sin \theta/\lambda)_{\max} = 0.68 \text{ \AA}^{-1}$. 7712 Reflections were unique ($R_{\text{int}} = 0.0522$), of which 5909 were observed [$I > 2\sigma(I)$]. 367 Parameters were refined. $R1/wR2$ [$I > 2\sigma(I)$]: 0.0352/0.0937. $R1/wR2$ [all refl.]: 0.0497/0.0974. $S = 1.018$. Residual electron density found between -0.63 and $0.80 \text{ e \AA}^{-3}$.

References:

- (1) Sheldrick, G. M. *Acta Cryst.* **2008**, *64*, 112-122
- (2) Spek, A. L. *Acta Cryst.* **2009**, *65*, 148-155.

DFT Data:

Table S1: Absolute energies, zero-point energies and free energies of DFT calculated structures. Also given are dispersion corrected energies (E_{disp}) and solvent energy (E_{solv}). Geometries optimized at UB3LYP/B1.

	E (B1)	ZPE (B1)	G (B1)	E_{solv}	E (B2)	E_{disp} (B2)
Nickel(II) Complexes						
¹ 5	-1778.285310	0.518848	-1777.828539	-45.7729	-1778.896295	-1777.390861
³ 5	-1778.275937	0.517597	-1777.821860	-45.1618	-1778.888356	-1777.370593
⁵ 5	-1778.225293	0.516065	-1777.774736	-39.5319	-1778.840463	-1777.313815
² [Ni ^{III} (LN ₃ S)] ⁰	-1778.473189	0.516086	-1778.017698	-13.4556	-1779.091135	-1778.473189
Iron(II) Complexes						
¹ 3	-2114.598946	0.684178	-2113.986084	-44.0630	-2115.392667	-2113.402611
³ 3	-2114.603486	0.684355	-2113.993085	-44.5044	-2115.397990	-2113.420448
⁵ 3	-2114.621034	0.683054	-2114.015586	-46.0380	-2115.418699	-2113.453619
⁴ 4	-2114.762060	0.679341	-2114.159079	-17.8990	-2115.566541	-2113.597691
² 4	-2114.775209	0.681040	-2114.170098	-18.1525	-2115.578244	-2113.600308

a. In au.

b. In kcal mol⁻¹.

Table S2: Relative energies (in kcal mol⁻¹) for iron and nickel complexes. Geometries optimized at UB3LYP/B1.

	ΔE (B1)	$\Delta E + \text{ZPE}$ (B1)	ΔE (B2)	$\Delta E + \text{ZPE}$ (B2)	ΔG (B1)	ΔG (B2)	ΔE_{disp}	$\Delta E_{\text{disp}} + \text{ZPE}$	$\Delta E + \text{ZPE} + E_{\text{solv}}$
Nickel(II) Complexes									
¹ 5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
³ 5	5.88	5.10	4.98	4.20	4.19	3.29	12.72	11.93	4.81
⁵ 5	37.66	35.92	35.03	33.29	33.76	31.13	48.35	46.60	39.53
² [Ni ^{III} (LN ₃ S)] ⁰	-117.90	-119.63	-122.26	-124.00	-118.70	-123.07	-679.17	-680.91	-91.68
Iron(II) Complexes									
¹ 3	13.86	14.57	16.34	17.04	18.51	20.99	32.01	32.71	19.02
³ 3	11.01	11.83	13.00	13.81	14.12	16.10	20.81	21.63	15.34
⁵ 3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
⁴ 4	-102.36	-105.39	-109.11	-112.14	-108.56	-115.31	-122.41	-125.45	-85.98
² 4	-110.61	-112.58	-116.45	-118.42	-115.47	-121.32	-124.06	-126.03	-92.51

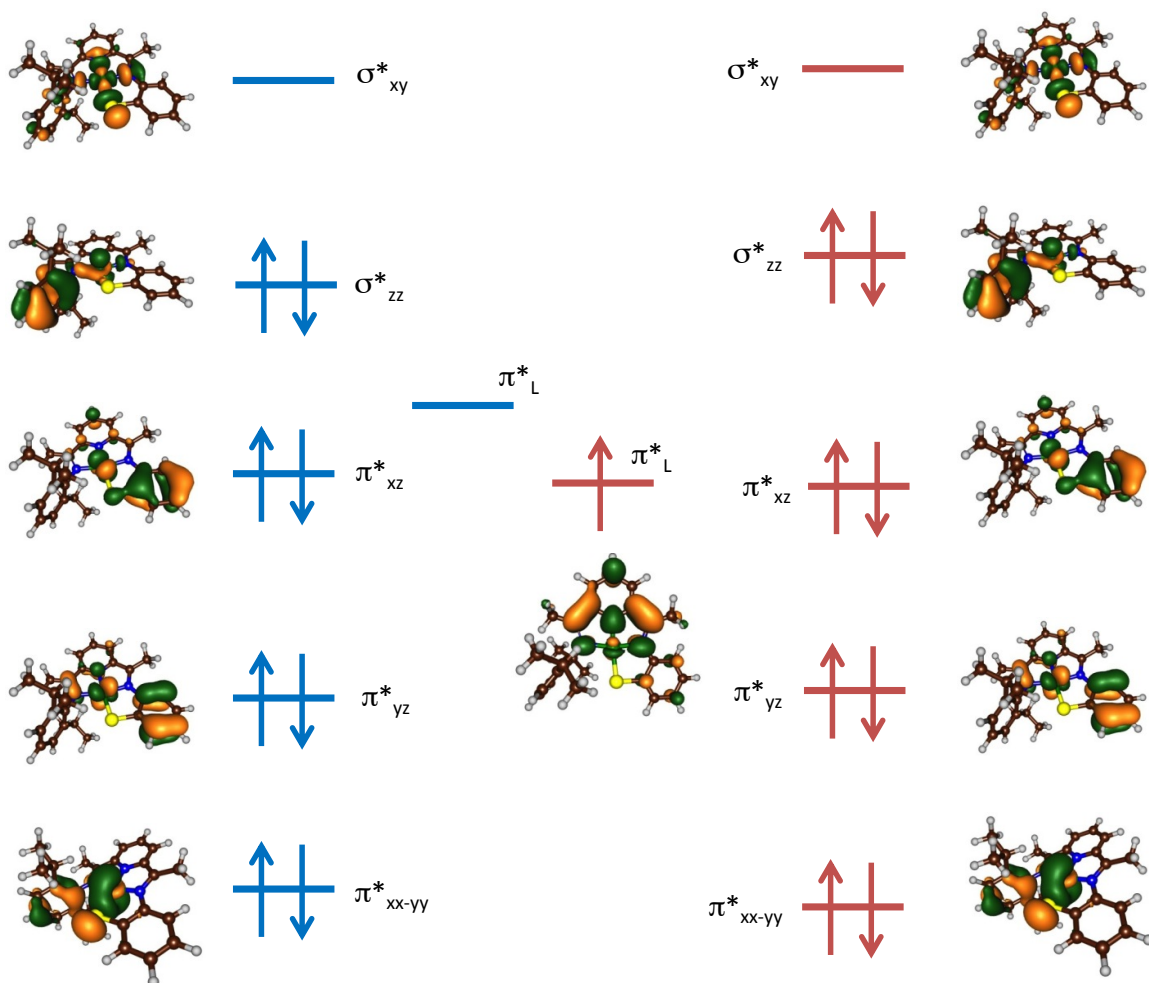


Figure S8. Orbital diagram of $1[\text{Ni}^{\text{II}}(\text{LN}_3\text{S})]^+$ (left-hand-side) and $2[\text{Ni}^{\text{II}}(\text{LN}_3\text{S})]^0$ (right-hand-side).

Table S3. Cartesian coordinates of all structures:

13:

26	-0.057725000	0.104267000	0.093772000
16	-0.638085000	0.607789000	2.247171000
6	1.070785000	0.431960000	2.887571000
6	1.425977000	0.951851000	4.138232000
6	2.751008000	0.888360000	4.581767000
6	3.741692000	0.317893000	3.769575000
6	3.401440000	-0.223880000	2.529314000
6	2.060865000	-0.196822000	2.090196000
6	2.121316000	-1.676142000	0.122147000
6	3.271346000	-2.561183000	0.515648000
6	1.377938000	-1.949687000	-1.117295000
6	1.654153000	-2.910400000	-2.102678000
6	0.759928000	-3.064087000	-3.170190000
6	-0.408909000	-2.289958000	-3.237467000
6	-0.645446000	-1.344345000	-2.232962000
6	-1.833494000	-0.485111000	-2.055236000
6	-2.956739000	-0.563138000	-3.048828000
6	-2.949941000	1.108247000	-0.622223000
6	-3.101989000	2.394170000	-1.194134000
6	-4.212599000	3.159976000	-0.800368000
6	-5.138557000	2.675040000	0.121238000
6	-4.966602000	1.405730000	0.674506000
6	-3.875531000	0.596394000	0.324127000
6	-2.115826000	2.987160000	-2.203395000
6	-2.774550000	3.220714000	-3.584751000
6	-1.500768000	4.305840000	-1.679482000
6	-3.753185000	-0.810461000	0.916302000
6	-4.670619000	-1.810346000	0.168969000
6	-4.046582000	-0.849790000	2.432328000
6	1.444834000	1.600911000	-2.069002000
6	2.222917000	2.611550000	-2.605859000
6	2.593584000	3.729375000	-1.804220000
6	2.119431000	3.716173000	-0.461442000
6	1.340674000	2.668156000	-0.005668000
6	3.826500000	4.726824000	-3.687526000
6	3.703107000	5.896792000	-1.439151000
7	1.604649000	-0.690025000	0.837876000
7	0.261014000	-1.179242000	-1.234941000
7	-1.810335000	0.268742000	-0.978150000
7	0.990237000	1.603951000	-0.786307000
7	3.354822000	4.753193000	-2.295684000
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1	3.014164000	1.300000000	5.550429000
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1	3.330885000	-2.664726000	1.601803000
1	4.234658000	-2.168134000	0.165009000
1	3.150409000	-3.559866000	0.088662000
1	2.540097000	-3.528866000	-2.040128000
1	0.964155000	-3.798330000	-3.940553000
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1	-1.294819000	2.276907000	-2.339616000
1	-2.038929000	3.611726000	-4.298068000

1	-3.193410000	2.297604000	-4.000060000
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1	1.166267000	0.752279000	-2.679500000
1	2.537509000	2.532743000	-3.637124000
1	2.345337000	4.523644000	0.220635000
1	0.961289000	2.658228000	1.006802000
1	4.468029000	3.857399000	-3.876915000
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1	2.988025000	4.705714000	-4.394655000
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6	2.523494000	3.104588000	-1.573040000
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6	1.191421000	4.066134000	0.200515000
6	0.547405000	2.846967000	0.321890000
6	3.952204000	5.566493000	-1.913458000
6	2.558157000	6.571425000	-0.046546000
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1	5.365257000	0.482126000	2.917005000
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1	-5.813639000	-0.619670000	0.983844000
1	-3.695297000	-0.624829000	3.380867000
1	-3.064998000	0.995112000	3.055061000
1	-4.815688000	0.684778000	2.995483000
1	2.067767000	1.049913000	-1.983442000
1	3.290134000	3.145904000	-2.334196000
1	0.895490000	4.874145000	0.854580000
1	-0.223850000	2.694816000	1.065371000
1	4.778711000	4.870641000	-1.722766000
1	4.347878000	6.580927000	-1.873635000
1	3.571389000	5.390312000	-2.926974000
1	3.193217000	7.414673000	-0.316467000
1	2.730589000	6.338859000	1.011357000
1	1.512786000	6.878367000	-0.172491000

53:

26	-0.002937000	-0.009402000	0.016732000
16	-0.010515000	0.022503000	2.423179000
6	1.815407000	-0.002461000	2.525723000
6	2.482175000	0.563832000	3.622835000
6	3.877142000	0.543765000	3.700360000
6	4.639564000	-0.039477000	2.675777000
6	3.999291000	-0.625726000	1.585451000
6	2.590312000	-0.619976000	1.505144000
6	2.074598000	-2.225936000	-0.265420000
6	3.167980000	-3.228769000	-0.006104000
6	1.054394000	-2.508046000	-1.304523000
6	1.104353000	-3.582449000	-2.210968000
6	0.042612000	-3.768851000	-3.098299000
6	-1.057721000	-2.900296000	-3.070353000
6	-1.050698000	-1.838941000	-2.156880000

6	-2.147476000	-0.834983000	-2.021944000
6	-3.378168000	-0.997325000	-2.871374000
6	-2.875635000	1.216101000	-0.962907000
6	-2.944341000	2.255972000	-1.928610000
6	-3.784970000	3.347459000	-1.651084000
6	-4.532038000	3.413833000	-0.475999000
6	-4.449912000	2.380196000	0.459256000
6	-3.622482000	1.268319000	0.244350000
6	-2.136334000	2.266991000	-3.233046000
6	-3.055472000	2.283778000	-4.479913000
6	-1.156167000	3.462535000	-3.289426000
6	-3.594279000	0.117608000	1.253085000
6	-4.736464000	-0.891641000	0.966569000
6	-3.652818000	0.589552000	2.721378000
6	1.839896000	2.121469000	-1.156229000
6	2.450726000	3.355329000	-1.283499000
6	1.935735000	4.480524000	-0.575114000
6	0.786772000	4.241305000	0.236289000
6	0.241752000	2.974291000	0.312227000
6	3.701949000	5.924011000	-1.505689000
6	1.956409000	6.850818000	0.086831000
7	1.858101000	-1.130907000	0.410713000
7	-0.004008000	-1.661092000	-1.320552000
7	-1.958626000	0.109743000	-1.147375000
7	0.744835000	1.905466000	-0.373201000
7	2.509523000	5.716623000	-0.668492000
1	1.895140000	1.022572000	4.409847000
1	4.373224000	0.992215000	4.554626000
1	5.722792000	-0.030554000	2.726451000
1	4.587818000	-1.044300000	0.776887000
1	3.541632000	-3.131123000	1.015441000
1	4.020054000	-3.093422000	-0.685700000
1	2.800644000	-4.251002000	-0.137023000
1	1.952077000	-4.254732000	-2.221924000
1	0.065413000	-4.590094000	-3.805358000
1	-1.890947000	-3.049790000	-3.743752000
1	-3.797051000	-2.003047000	-2.746984000
1	-3.145179000	-0.866602000	-3.935076000
1	-4.141171000	-0.268777000	-2.597251000
1	-3.853025000	4.156118000	-2.371224000
1	-5.177731000	4.265748000	-0.289629000
1	-5.037502000	2.435921000	1.368213000
1	-1.528720000	1.356255000	-3.278670000
1	-2.455842000	2.216239000	-5.395806000
1	-3.769538000	1.454825000	-4.475630000
1	-3.632071000	3.213462000	-4.530723000
1	-0.557857000	3.417484000	-4.207916000
1	-0.475530000	3.464148000	-2.433715000
1	-1.699188000	4.413907000	-3.291780000
1	-2.644042000	-0.416307000	1.124851000
1	-4.681009000	-1.735368000	1.664601000
1	-4.683723000	-1.289135000	-0.054555000
1	-5.716072000	-0.412557000	1.088247000
1	-3.500613000	-0.264241000	3.390716000
1	-2.869582000	1.323454000	2.936874000
1	-4.625208000	1.030972000	2.970277000
1	2.228856000	1.260738000	-1.685520000
1	3.320465000	3.445331000	-1.919427000
1	0.332186000	5.035178000	0.810852000
1	-0.611728000	2.776713000	0.948187000
1	4.544614000	5.313527000	-1.160633000

1	3.998280000	6.970677000	-1.451655000
1	3.499138000	5.683283000	-2.555878000
1	2.552160000	7.739219000	-0.121288000
1	1.985389000	6.665017000	1.167336000
1	0.920458000	7.058387000	-0.205645000

24:

26	3.405019000	9.865004000	8.809484000
16	4.305090000	9.362658000	6.688066000
6	6.007685000	9.776179000	7.193207000
6	7.010347000	10.001495000	6.234513000
1	6.759229000	9.880987000	5.185992000
6	8.296368000	10.393116000	6.614375000
1	9.053952000	10.569279000	5.856111000
6	8.599308000	10.583781000	7.970624000
1	9.584428000	10.926814000	8.271168000
6	7.623925000	10.344196000	8.940599000
1	7.858987000	10.535113000	9.979152000
6	6.331295000	9.908963000	8.572368000
6	5.382223000	9.244332000	10.750912000
6	6.665084000	8.889367000	11.457438000
1	7.383385000	8.442192000	10.763122000
1	6.469884000	8.165629000	12.251631000
1	7.150576000	9.758922000	11.918101000
6	4.103776000	9.042603000	11.405828000
6	3.845028000	8.631016000	12.716456000
1	4.656022000	8.466619000	13.414975000
6	2.510574000	8.426585000	13.124975000
1	2.304751000	8.106735000	14.140462000
6	1.453597000	8.615506000	12.227644000
1	0.430767000	8.433949000	12.537955000
6	1.731261000	9.031971000	10.915763000
6	0.824386000	9.232240000	9.822108000
6	-0.652915000	8.980382000	9.992117000
1	-1.093958000	9.678241000	10.716501000
1	-0.838931000	7.966359000	10.368860000
1	-1.188300000	9.092885000	9.048505000
6	0.621365000	9.775092000	7.467905000
6	-0.025678000	11.005985000	7.187737000
6	-0.782509000	11.114822000	6.008743000
1	-1.285868000	12.050805000	5.786083000
6	-0.902807000	10.045098000	5.123723000
1	-1.494177000	10.147946000	4.218427000
6	-0.257204000	8.841474000	5.407612000
1	-0.351388000	8.011232000	4.715934000
6	0.512678000	8.679123000	6.570544000
6	0.059241000	12.209028000	8.129455000
1	0.772450000	11.960228000	8.920809000
6	-1.305853000	12.516475000	8.792412000
1	-2.057006000	12.783810000	8.038226000
1	-1.213886000	13.361315000	9.487193000
1	-1.686141000	11.655408000	9.351472000
6	0.589119000	13.467512000	7.405464000
1	1.545115000	13.265254000	6.915258000
1	0.737028000	14.284156000	8.122740000
1	-0.117144000	13.817323000	6.642261000
6	1.170522000	7.326470000	6.858507000
1	1.917181000	7.483563000	7.643670000
6	0.134309000	6.302057000	7.383303000
1	-0.371594000	6.661508000	8.285303000
1	0.626917000	5.352093000	7.625564000

1	-0.633109000	6.101317000	6.624294000
6	1.913063000	6.750222000	5.633525000
1	1.222422000	6.489427000	4.821628000
1	2.444321000	5.834605000	5.920570000
1	2.650347000	7.461745000	5.254168000
6	4.193715000	12.731648000	7.856091000
1	4.420849000	12.165371000	6.961638000
6	4.457947000	14.091826000	7.936538000
1	4.902655000	14.585189000	7.083424000
6	4.142738000	14.809053000	9.120027000
6	3.567432000	14.055708000	10.177874000
1	3.300637000	14.518867000	11.117772000
6	3.342538000	12.696694000	10.012663000
1	2.908057000	12.109492000	10.813074000
6	4.987432000	16.900329000	8.126864000
1	5.987421000	16.517443000	7.884609000
1	5.083997000	17.949534000	8.407080000
1	4.370320000	16.845986000	7.221194000
6	4.045609000	16.863836000	10.477347000
1	2.976212000	16.781939000	10.711093000
1	4.285715000	17.921289000	10.363860000
1	4.615006000	16.473836000	11.331796000
7	5.270514000	9.657233000	9.481897000
7	3.045861000	9.262877000	10.546351000
7	1.414748000	9.620788000	8.669556000
7	3.639493000	12.021621000	8.873309000
7	4.379679000	16.161892000	9.236576000

44:

26	3.400952000	9.807009000	8.788791000
16	4.358193000	9.360841000	6.682691000
6	6.037748000	9.805906000	7.236227000
6	7.055657000	10.068569000	6.304977000
1	6.832386000	9.956321000	5.249382000
6	8.320539000	10.492353000	6.719986000
1	9.089754000	10.700954000	5.982238000
6	8.584157000	10.676662000	8.084658000
1	9.550229000	11.047290000	8.412551000
6	7.593992000	10.396208000	9.028359000
1	7.797468000	10.584345000	10.074080000
6	6.324450000	9.927634000	8.624438000
6	5.350379000	9.237446000	10.782240000
6	6.626595000	8.884311000	11.503079000
1	7.363905000	8.469051000	10.809954000
1	6.429339000	8.134886000	12.274206000
1	7.090759000	9.748771000	11.997329000
6	4.064516000	9.052580000	11.427245000
6	3.799515000	8.665171000	12.745473000
1	4.605367000	8.495960000	13.449167000
6	2.457974000	8.495587000	13.148124000
1	2.239091000	8.205814000	14.169897000
6	1.406477000	8.675564000	12.238703000
1	0.381669000	8.516215000	12.554348000
6	1.692726000	9.051603000	10.916755000
6	0.788996000	9.214835000	9.810523000
6	-0.687454000	8.967184000	9.990671000
1	-1.169278000	9.790873000	10.535434000
1	-0.866049000	8.051211000	10.565443000
1	-1.191346000	8.870323000	9.028169000
6	0.561419000	9.730055000	7.444128000
6	-0.098173000	10.955802000	7.165349000

6	-0.865016000	11.055703000	5.993093000
1	-1.377749000	11.987252000	5.772492000
6	-0.978555000	9.983891000	5.108145000
1	-1.579377000	10.078999000	4.208534000
6	-0.309110000	8.790593000	5.381741000
1	-0.391139000	7.962205000	4.685829000
6	0.471599000	8.638804000	6.538599000
6	0.007717000	12.167748000	8.094015000
1	0.714101000	11.913818000	8.889793000
6	-1.350378000	12.516988000	8.748384000
1	-2.086999000	12.811128000	7.990725000
1	-1.235901000	13.355967000	9.446756000
1	-1.764047000	11.667099000	9.300769000
6	0.570049000	13.403505000	7.354106000
1	1.525886000	13.173187000	6.876139000
1	0.729092000	14.229653000	8.058487000
1	-0.122135000	13.753895000	6.578887000
6	1.176434000	7.307332000	6.811065000
1	1.925962000	7.486192000	7.588847000
6	0.184603000	6.244765000	7.345004000
1	-0.313956000	6.579561000	8.260949000
1	0.711634000	5.308752000	7.567909000
1	-0.591128000	6.027094000	6.599857000
6	1.927623000	6.766594000	5.575221000
1	1.239093000	6.490426000	4.767237000
1	2.492796000	5.867501000	5.848422000
1	2.637428000	7.505764000	5.195177000
6	4.163511000	12.766657000	7.829291000
1	4.308136000	12.198774000	6.918333000
6	4.446499000	14.124967000	7.885750000
1	4.818086000	14.616876000	6.997350000
6	4.244133000	14.841946000	9.093781000
6	3.759457000	14.091533000	10.198915000
1	3.581049000	14.556275000	11.158864000
6	3.510231000	12.733511000	10.051444000
1	3.148834000	12.145202000	10.887600000
6	4.992729000	16.933847000	8.022404000
1	5.952081000	16.538101000	7.665194000
1	5.139563000	17.978312000	8.297834000
1	4.276403000	16.898352000	7.191105000
6	4.294501000	16.894684000	10.457903000
1	3.248034000	16.836176000	10.787366000
1	4.550264000	17.946950000	10.329172000
1	4.928143000	16.484634000	11.256298000
7	5.251234000	9.644679000	9.509681000
7	3.016340000	9.269279000	10.567942000
7	1.357814000	9.591115000	8.638818000
7	3.696298000	12.058646000	8.889989000
7	4.502254000	16.193577000	9.189168000

15:

28	-0.007258000	0.013535000	-0.005032000
16	-0.034175000	0.028760000	2.196102000
7	1.932508000	0.021646000	-0.039660000
7	0.164247000	0.096180000	-1.843929000
7	-1.907010000	-0.009153000	-0.440267000
6	1.778314000	-0.070714000	2.352748000
6	2.354570000	-0.154498000	3.626107000
6	3.733003000	-0.320451000	3.769271000
6	4.553612000	-0.422559000	2.634409000
6	4.001681000	-0.318815000	1.361303000

6	2.609358000	-0.106397000	1.200469000
6	2.435100000	0.209484000	-1.253269000
6	3.871753000	0.453497000	-1.607753000
6	1.416977000	0.207713000	-2.331545000
6	1.581520000	0.298749000	-3.721988000
6	0.436039000	0.278835000	-4.535721000
6	-0.849601000	0.182247000	-3.981653000
6	-0.956658000	0.094596000	-2.587291000
6	-2.164611000	0.015879000	-1.728594000
6	-3.527957000	-0.020897000	-2.345063000
6	-2.964520000	-0.080126000	0.558920000
6	-3.405528000	-1.351881000	0.994310000
6	-4.418794000	-1.385612000	1.965007000
6	-4.957969000	-0.210635000	2.490223000
6	-4.481724000	1.029604000	2.063479000
6	-3.469042000	1.127294000	1.096435000
6	-2.813923000	-2.661774000	0.467406000
6	-2.172442000	-3.488066000	1.607657000
6	-3.867957000	-3.499334000	-0.295488000
6	-2.951131000	2.503780000	0.671597000
6	-2.410360000	3.305732000	1.879076000
6	-4.034929000	3.309508000	-0.084225000
1	1.713305000	-0.110220000	4.498792000
1	4.165831000	-0.393421000	4.761117000
1	5.618395000	-0.591907000	2.744315000
1	4.652202000	-0.443880000	0.510899000
1	4.348298000	1.115448000	-0.879100000
1	3.950284000	0.927025000	-2.588305000
1	4.451965000	-0.477789000	-1.645145000
1	2.563596000	0.377607000	-4.168826000
1	0.549433000	0.344485000	-5.611485000
1	-1.727964000	0.178902000	-4.614011000
1	-4.307664000	-0.069287000	-1.586006000
1	-3.694113000	0.872471000	-2.960152000
1	-3.626410000	-0.893352000	-3.003338000
1	-4.782875000	-2.344741000	2.316864000
1	-5.741302000	-0.261584000	3.239004000
1	-4.895475000	1.936764000	2.490127000
1	-2.010369000	-2.417500000	-0.238414000
1	-1.409020000	-2.905144000	2.132455000
1	-2.923087000	-3.804478000	2.340346000
1	-1.703166000	-4.391442000	1.201056000
1	-4.307920000	-2.939289000	-1.129061000
1	-4.685832000	-3.802295000	0.367823000
1	-3.411693000	-4.410558000	-0.698364000
1	-2.108118000	2.355635000	-0.014672000
1	-1.625110000	2.749046000	2.399649000
1	-1.992486000	4.260544000	1.539519000
1	-3.205684000	3.529257000	2.598725000
1	-3.632122000	4.273236000	-0.415540000
1	-4.895862000	3.512511000	0.562597000
1	-4.402801000	2.770804000	-0.965553000
35:			
28	-0.034329000	-0.049379000	0.167310000
16	0.309679000	0.540273000	2.315832000
7	2.046871000	-0.190642000	-0.035840000
7	0.178235000	0.178023000	-1.783980000
7	-2.052486000	-0.004857000	-0.473926000
6	2.047184000	-0.032537000	2.359383000
6	2.688781000	-0.164349000	3.599448000

6	3.991522000	-0.660906000	3.674313000
6	4.675514000	-1.032778000	2.505692000
6	4.068853000	-0.876580000	1.261313000
6	2.758866000	-0.356474000	1.168901000
6	2.496125000	0.073055000	-1.238935000
6	3.928645000	0.319872000	-1.622367000
6	1.434147000	0.196132000	-2.277036000
6	1.616805000	0.334401000	-3.663403000
6	0.484215000	0.447520000	-4.479881000
6	-0.806735000	0.422225000	-3.928055000
6	-0.930418000	0.276943000	-2.541051000
6	-2.200298000	0.202891000	-1.753305000
6	-3.511552000	0.340824000	-2.469603000
6	-3.152246000	-0.083499000	0.463769000
6	-3.450643000	-1.355183000	1.013381000
6	-4.472272000	-1.431519000	1.969978000
6	-5.155108000	-0.288594000	2.390127000
6	-4.821765000	0.956854000	1.858568000
6	-3.816482000	1.094468000	0.886960000
6	-2.702480000	-2.624622000	0.599124000
6	-2.008999000	-3.295051000	1.809560000
6	-3.630481000	-3.624844000	-0.129276000
6	-3.437429000	2.494753000	0.395440000
6	-2.747878000	3.303994000	1.522213000
6	-4.649612000	3.270757000	-0.169696000
1	2.151897000	0.107671000	4.500896000
1	4.468665000	-0.774574000	4.641580000
1	5.674592000	-1.449039000	2.568349000
1	4.590840000	-1.203963000	0.371895000
1	4.488976000	0.735497000	-0.780840000
1	3.994405000	1.026165000	-2.453830000
1	4.432952000	-0.604607000	-1.933237000
1	2.607115000	0.348126000	-4.099328000
1	0.606704000	0.553823000	-5.551627000
1	-1.678987000	0.507816000	-4.562904000
1	-4.348760000	0.171787000	-1.792588000
1	-3.614858000	1.343549000	-2.903212000
1	-3.578144000	-0.380391000	-3.293348000
1	-4.731903000	-2.395251000	2.394848000
1	-5.938865000	-0.367970000	3.135925000
1	-5.342855000	1.841597000	2.207501000
1	-1.915811000	-2.340064000	-0.112541000
1	-1.328009000	-2.600536000	2.314161000
1	-2.743273000	-3.638259000	2.547186000
1	-1.434289000	-4.169234000	1.481488000
1	-4.099293000	-3.171723000	-1.010131000
1	-4.431517000	-3.974423000	0.531946000
1	-3.061985000	-4.503130000	-0.456209000
1	-2.708818000	2.396108000	-0.417961000
1	-1.859108000	2.788030000	1.901804000
1	-2.442087000	4.289207000	1.151215000
1	-3.431163000	3.458678000	2.365012000
1	-4.321328000	4.232116000	-0.580843000
1	-5.387945000	3.483857000	0.610726000
1	-5.157101000	2.712737000	-0.964462000
55:			
28	-0.016898000	0.039749000	0.112814000
16	0.220913000	0.081112000	2.463796000
7	2.017657000	0.019176000	0.003859000
7	0.178655000	0.107500000	-1.801310000

7	-2.023112000	0.003076000	-0.468471000
6	1.990944000	-0.099806000	2.426644000
6	2.660622000	-0.226591000	3.670977000
6	4.022995000	-0.453030000	3.722305000
6	4.744026000	-0.575024000	2.510397000
6	4.121945000	-0.437083000	1.273019000
6	2.735755000	-0.157107000	1.172075000
6	2.486506000	0.192896000	-1.288676000
6	3.921831000	0.439894000	-1.663350000
6	1.459196000	0.208372000	-2.289940000
6	1.602876000	0.314859000	-3.701753000
6	0.473722000	0.308349000	-4.508939000
6	-0.828719000	0.209616000	-3.949923000
6	-0.940758000	0.115169000	-2.569565000
6	-2.189465000	0.034064000	-1.770091000
6	-3.521795000	-0.003357000	-2.461031000
6	-3.118827000	-0.072989000	0.479540000
6	-3.542564000	-1.345502000	0.933531000
6	-4.561726000	-1.389069000	1.897819000
6	-5.131652000	-0.219602000	2.402672000
6	-4.681659000	1.023395000	1.956111000
6	-3.664742000	1.128019000	0.993739000
6	-2.920540000	-2.650406000	0.429932000
6	-2.233589000	-3.427023000	1.579392000
6	-3.959362000	-3.542097000	-0.291007000
6	-3.179692000	2.511243000	0.552415000
6	-2.601186000	3.315026000	1.741940000
6	-4.299382000	3.310840000	-0.156222000
1	2.073655000	-0.157769000	4.579535000
1	4.530411000	-0.555686000	4.673896000
1	5.807704000	-0.786705000	2.541174000
1	4.717798000	-0.567759000	0.384949000
1	4.403159000	1.124601000	-0.956861000
1	3.992720000	0.896696000	-2.652202000
1	4.516205000	-0.482901000	-1.692595000
1	2.584504000	0.388502000	-4.151781000
1	0.584210000	0.381773000	-5.584339000
1	-1.701604000	0.213388000	-4.589875000
1	-4.338765000	-0.060206000	-1.741689000
1	-3.662439000	0.893094000	-3.076724000
1	-3.584724000	-0.871098000	-3.128763000
1	-4.909518000	-2.351330000	2.258491000
1	-5.919302000	-0.276702000	3.146440000
1	-5.122458000	1.927907000	2.361659000
1	-2.142366000	-2.400362000	-0.302459000
1	-1.474235000	-2.813309000	2.078065000
1	-2.960167000	-3.737742000	2.338439000
1	-1.748511000	-4.330521000	1.192242000
1	-4.432264000	-3.013897000	-1.126654000
1	-4.753471000	-3.858309000	0.394728000
1	-3.479436000	-4.445608000	-0.683824000
1	-2.366449000	2.375158000	-0.171563000
1	-1.788465000	2.769814000	2.235462000
1	-2.209516000	4.278201000	1.395064000
1	-3.369910000	3.520505000	2.495211000
1	-3.917089000	4.277322000	-0.503575000
1	-5.135079000	3.508053000	0.524681000
1	-4.696884000	2.768378000	-1.021502000

$^2[\text{Ni}^{\text{III}}(\text{LN}_3\text{S})]_0$:

28	-0.013957000	0.025414000	-0.001634000
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16	-0.030839000	0.066877000	2.225441000
7	1.903410000	0.004452000	-0.027447000
7	0.161599000	0.106577000	-1.819808000
7	-1.901308000	-0.001277000	-0.449025000
6	1.776896000	-0.078168000	2.372997000
6	2.366997000	-0.180511000	3.640330000
6	3.742117000	-0.375657000	3.776297000
6	4.541731000	-0.489850000	2.630739000
6	3.974230000	-0.374275000	1.361892000
6	2.587739000	-0.132172000	1.205012000
6	2.430227000	0.177447000	-1.267187000
6	3.881966000	0.402079000	-1.593422000
6	1.441137000	0.191739000	-2.316281000
6	1.590815000	0.273054000	-3.710222000
6	0.450861000	0.262029000	-4.530013000
6	-0.843485000	0.183233000	-3.977280000
6	-0.970362000	0.109497000	-2.589004000
6	-2.159092000	0.047627000	-1.760808000
6	-3.537477000	0.039066000	-2.360865000
6	-2.961587000	-0.076050000	0.532491000
6	-3.393719000	-1.347751000	0.980472000
6	-4.410799000	-1.397039000	1.946245000
6	-4.973713000	-0.229828000	2.463970000
6	-4.514306000	1.014171000	2.030206000
6	-3.499673000	1.119886000	1.065699000
6	-2.769533000	-2.646943000	0.466896000
6	-2.074442000	-3.423196000	1.610653000
6	-3.805754000	-3.537605000	-0.258087000
6	-2.997492000	2.501368000	0.640277000
6	-2.398069000	3.276047000	1.837763000
6	-4.108246000	3.327303000	-0.051147000
1	1.729725000	-0.123992000	4.516313000
1	4.183500000	-0.459526000	4.764474000
1	5.606608000	-0.678378000	2.722593000
1	4.614256000	-0.506634000	0.504266000
1	4.341153000	1.102781000	-0.888567000
1	3.981936000	0.829203000	-2.594261000
1	4.472365000	-0.523797000	-1.572825000
1	2.575237000	0.335273000	-4.158418000
1	0.569228000	0.317564000	-5.606130000
1	-1.717858000	0.185236000	-4.617410000
1	-4.305623000	-0.015136000	-1.588739000
1	-3.710738000	0.945192000	-2.954991000
1	-3.664030000	-0.819928000	-3.032020000
1	-4.756781000	-2.362302000	2.302481000
1	-5.758698000	-0.289560000	3.211641000
1	-4.941099000	1.919092000	2.451190000
1	-1.992286000	-2.382198000	-0.257650000
1	-1.320049000	-2.796923000	2.097177000
1	-2.797096000	-3.744917000	2.370627000
1	-1.581647000	-4.320186000	1.215116000
1	-4.278907000	-3.007080000	-1.092978000
1	-4.600439000	-3.860227000	0.425709000
1	-3.321964000	-4.438271000	-0.655382000
1	-2.188512000	2.356081000	-0.083457000
1	-1.587099000	2.704341000	2.299505000
1	-1.996706000	4.240171000	1.501365000
1	-3.157489000	3.478063000	2.603098000
1	-3.712025000	4.293711000	-0.385925000
1	-4.939287000	3.527226000	0.636349000
1	-4.516306000	2.804219000	-0.92408000